

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
 Data File : BM033544.D
 Acq On : 20 Dec 2021 17:32
 Operator : CG/JU
 Sample : M5079-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 338

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.625	62	66	79	rBV	216030	292786	20.45%	3.460%
2	5.025	299	304	311	rBV	66437	98204	6.86%	1.161%
3	5.484	375	382	400	rBV	535239	817691	57.11%	9.664%
4	7.090	648	655	673	rBV	529144	918492	64.15%	10.856%
5	7.919	790	796	805	rBV	123221	193378	13.51%	2.286%
6	9.096	988	996	1010	rBV	335944	592456	41.38%	7.002%
7	10.525	1233	1239	1251	rBV2	18233	46804	3.27%	0.553%
8	10.731	1267	1274	1281	rBV	142756	250390	17.49%	2.959%
9	13.189	1686	1692	1704	rVB	737036	1120295	78.24%	13.241%
10	13.531	1745	1750	1760	rBV3	9327	26294	1.84%	0.311%
11	14.213	1862	1866	1875	rBV4	12245	19510	1.36%	0.231%
12	14.566	1921	1926	1935	rVB	213805	311731	21.77%	3.684%
13	16.060	2174	2180	2195	rVB	549232	808884	56.49%	9.560%
14	17.230	2374	2379	2385	rVB2	18367	21854	1.53%	0.258%
15	17.319	2385	2394	2399	rBV	233740	347480	24.27%	4.107%
16	17.601	2438	2442	2450	rBV2	11083	17461	1.22%	0.206%
17	18.207	2540	2545	2550	rBV2	43426	63902	4.46%	0.755%
18	18.283	2555	2558	2565	rVB	16019	21833	1.52%	0.258%
19	19.371	2739	2743	2748	rVB	22837	34080	2.38%	0.403%
20	19.483	2756	2762	2767	rBV10	13777	23874	1.67%	0.282%
21	19.736	2802	2805	2811	rVB	19146	24952	1.74%	0.295%
22	19.936	2833	2839	2845	rBV	1189587	1431879	100.00%	16.923%
23	20.548	2939	2943	2953	rBV	23714	60726	4.24%	0.718%
24	21.195	3050	3053	3063	rVB3	69028	106604	7.45%	1.260%
25	21.495	3099	3104	3109	rBV	252978	339832	23.73%	4.016%
26	21.842	3160	3163	3171	rBV	41277	75240	5.25%	0.889%
27	22.742	3313	3316	3322	rVB2	48903	70984	4.96%	0.839%
28	23.901	3507	3513	3523	rVB	156516	323447	22.59%	3.823%

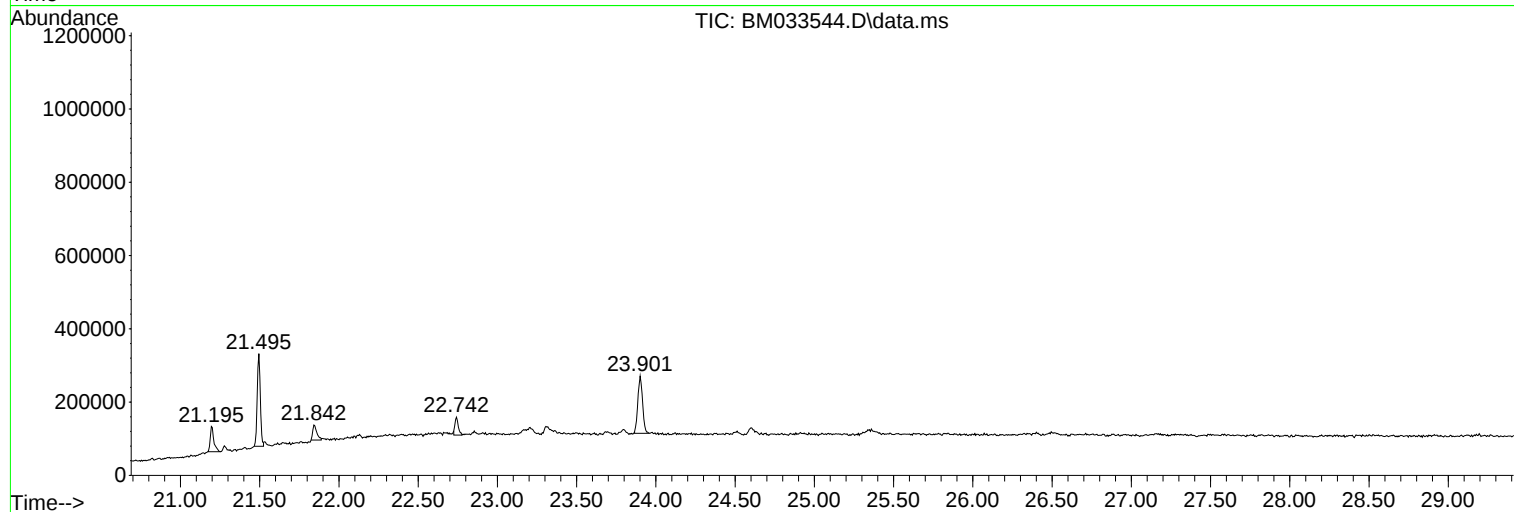
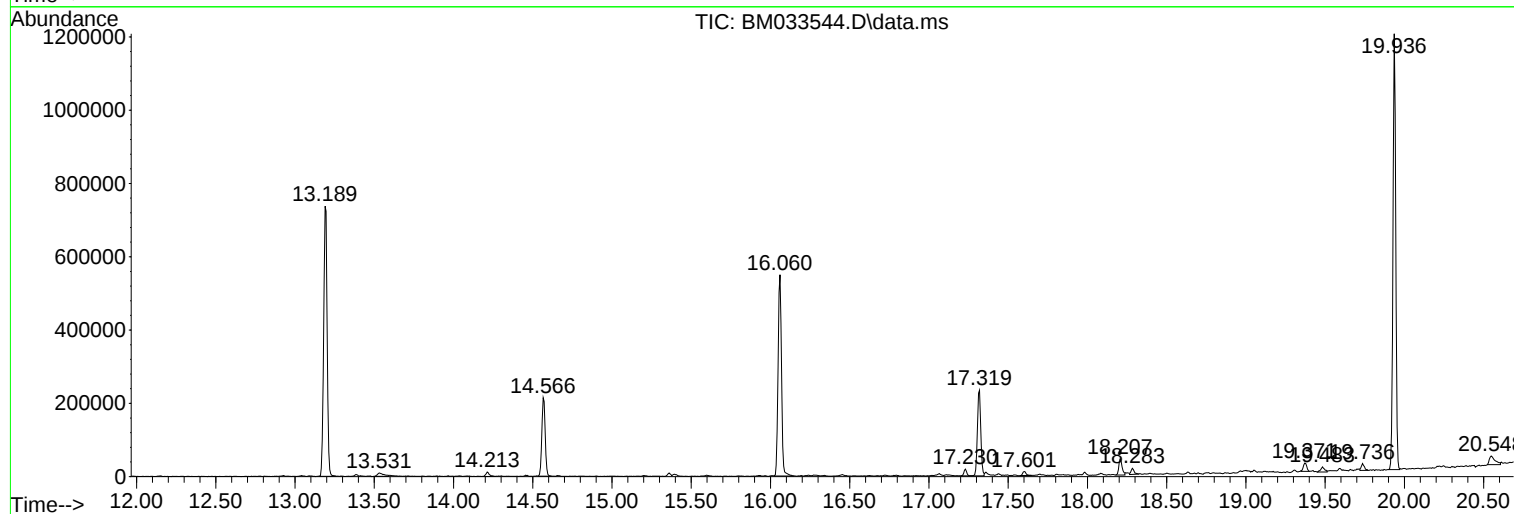
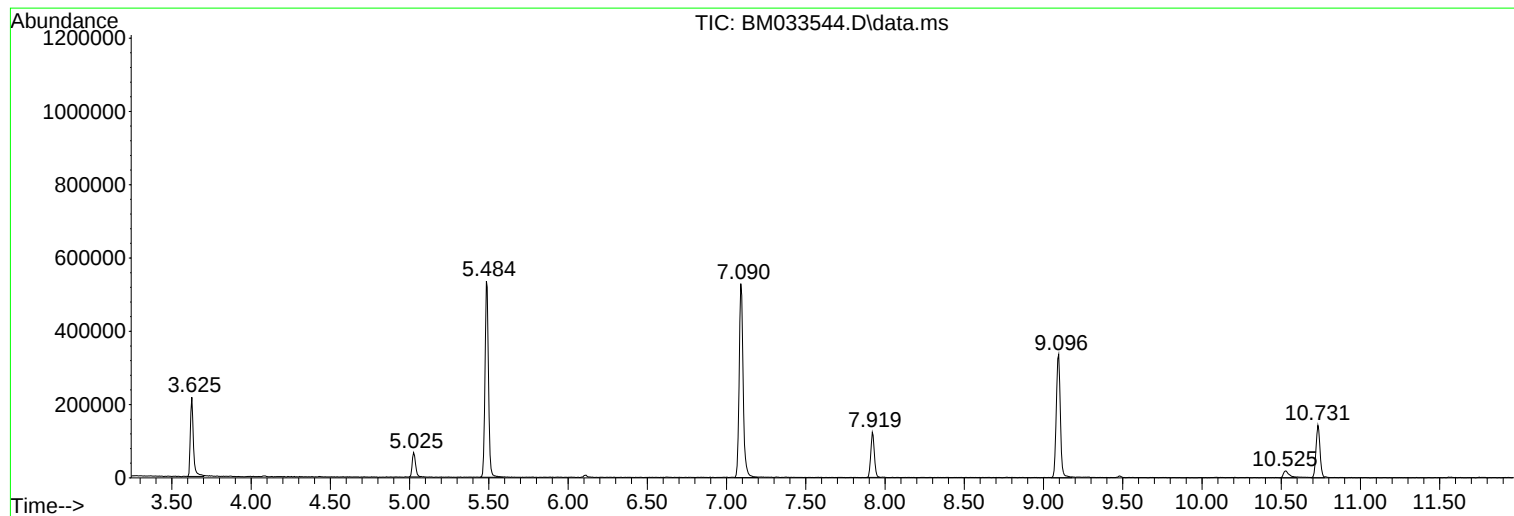
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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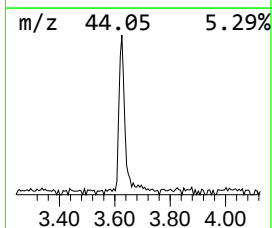
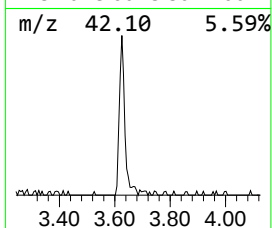
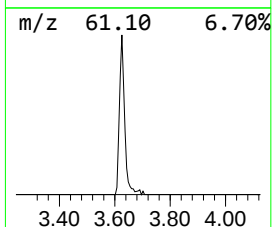
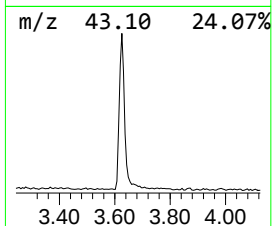
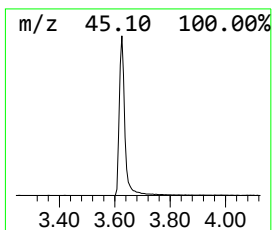
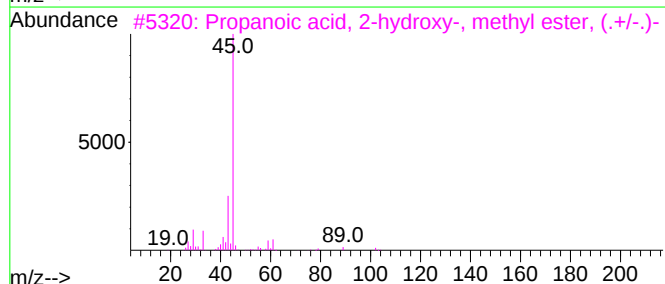
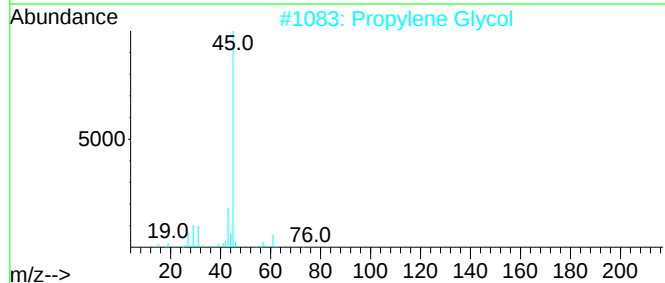
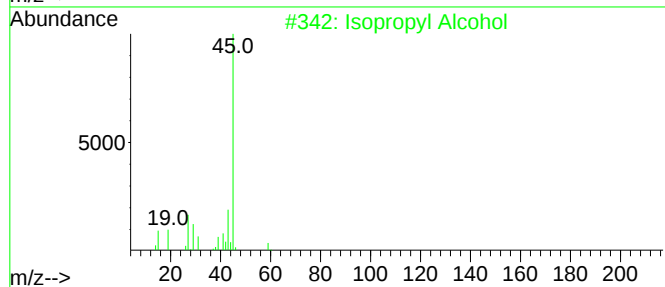
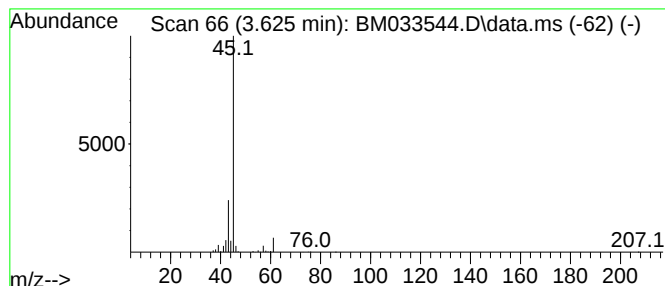
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.625	30.28 ng	292786	1,4-Dichlorobenzene-d4	7.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Propylene Glycol	76	C3H8O2	000057-55-6	38
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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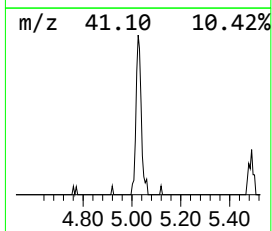
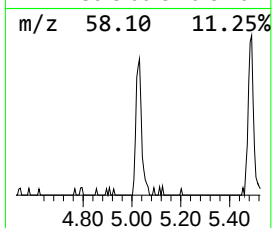
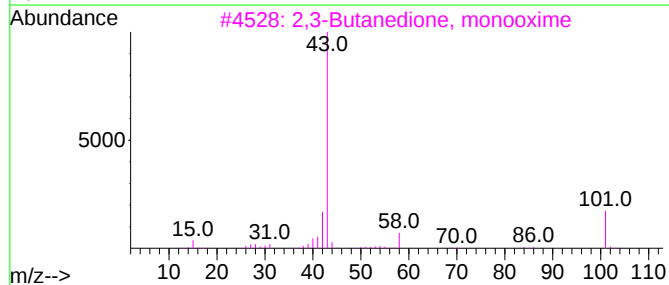
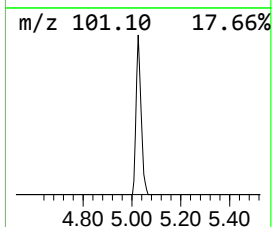
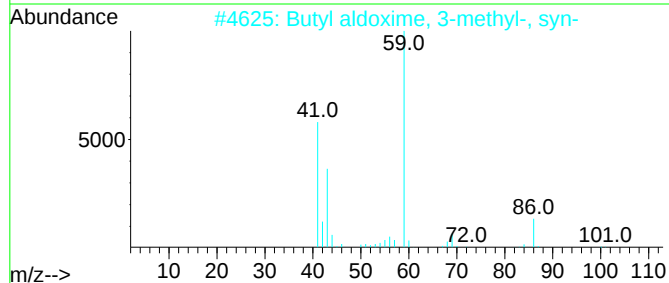
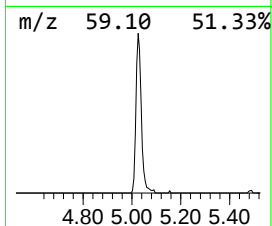
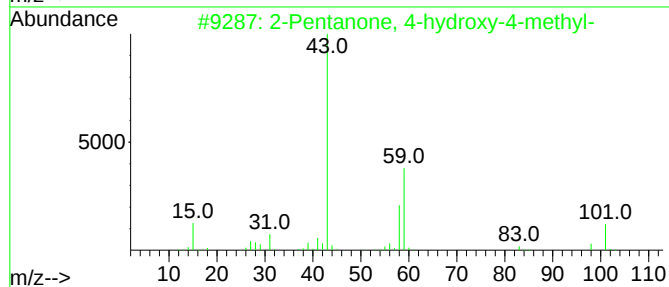
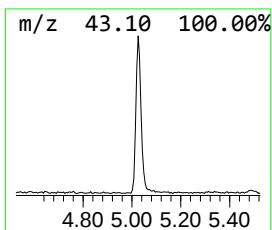
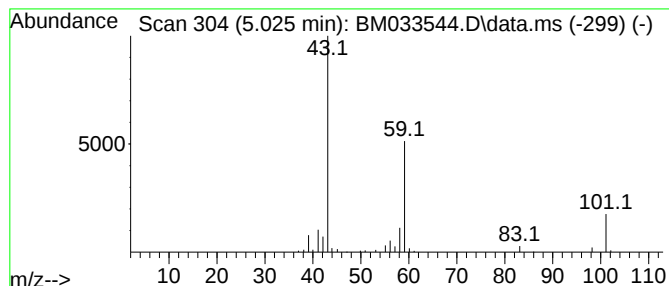
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.025	10.16 ng	98204	1,4-Dichlorobenzene-d4	7.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Butane	58	C4H10	000106-97-8	9
5			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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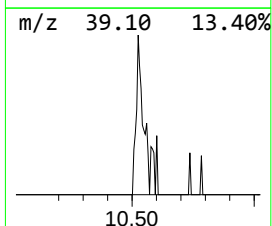
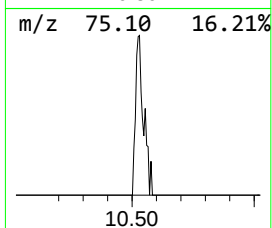
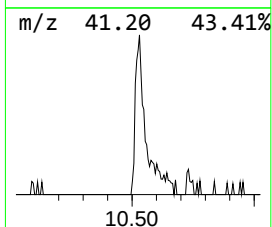
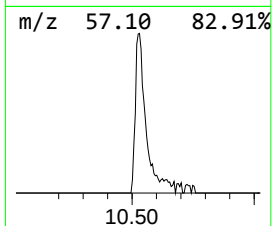
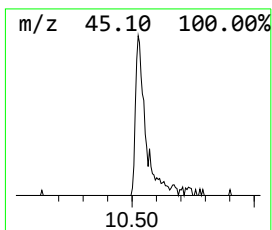
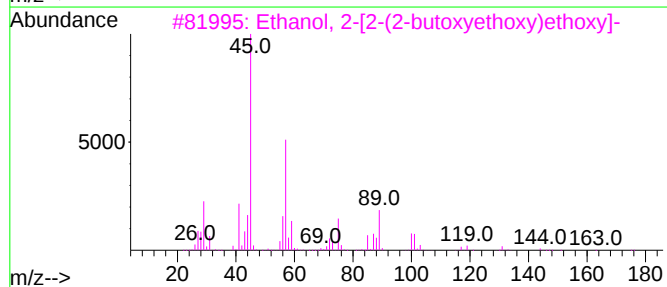
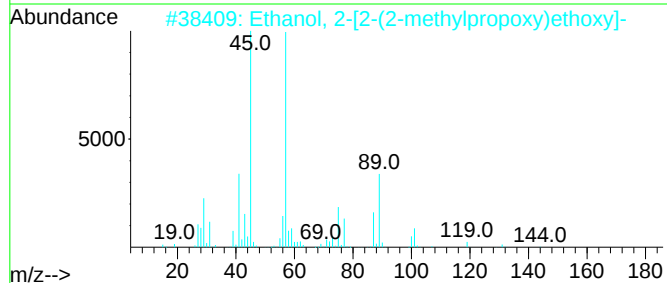
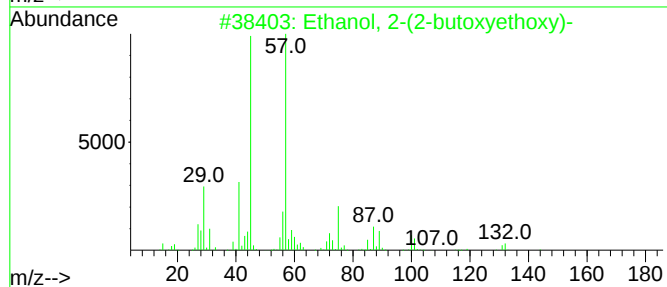
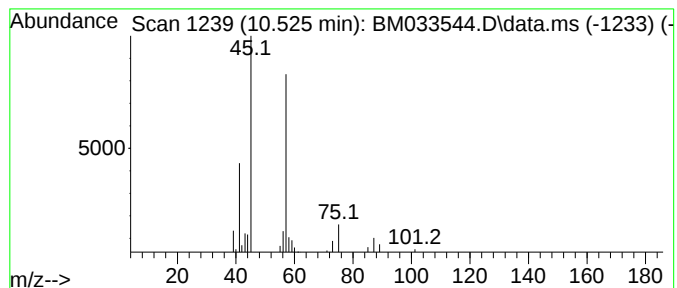
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.525	3.74 ng	46804	Naphthalene-d8	10.731

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	38
5			Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	33



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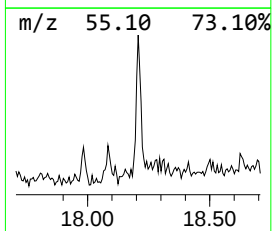
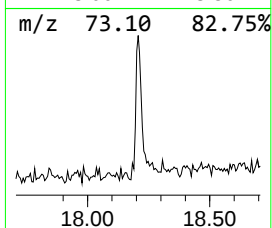
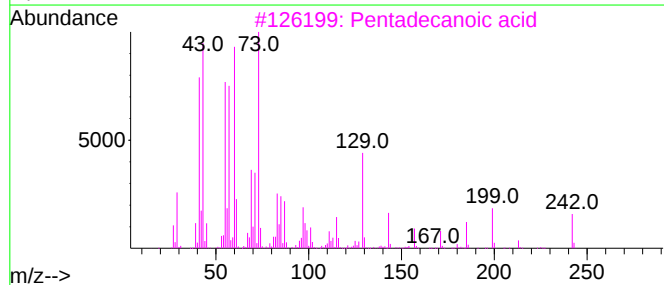
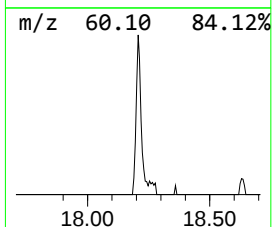
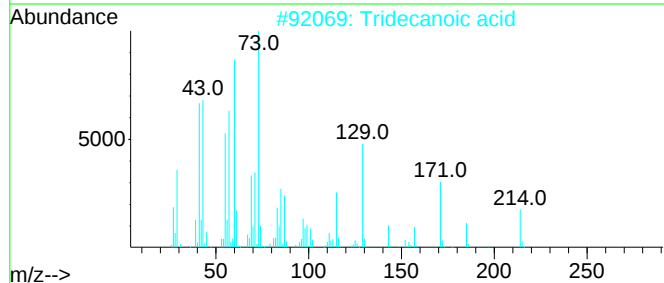
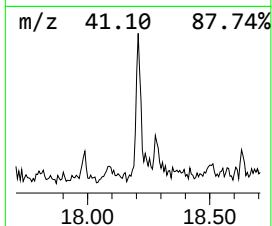
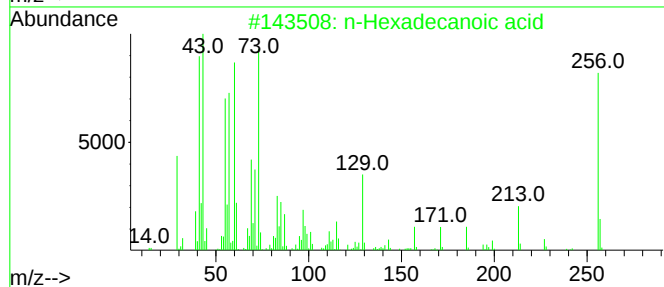
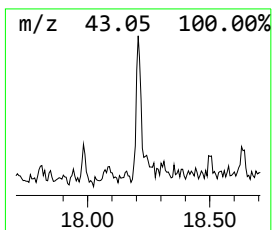
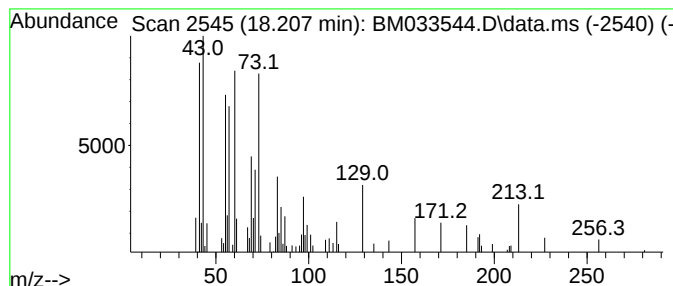
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.207	3.68 ng	63902	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Undecanoic acid	186	C11H22O2	000112-37-8	59
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58



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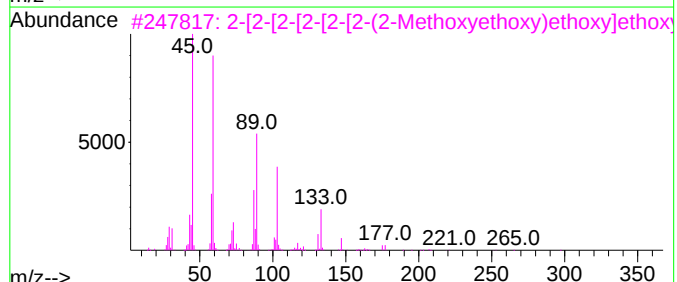
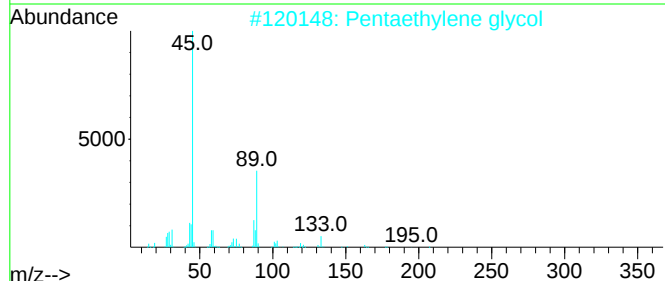
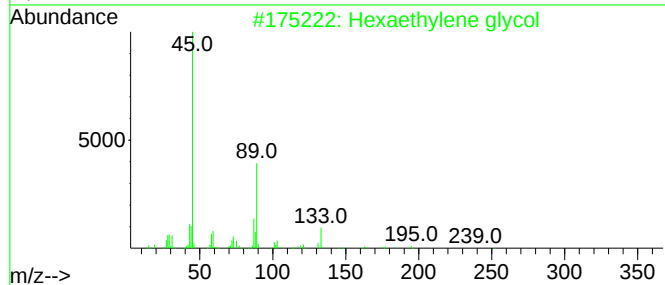
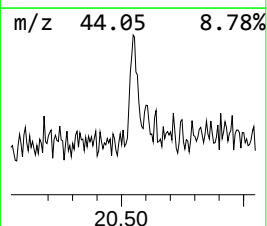
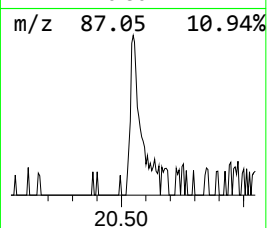
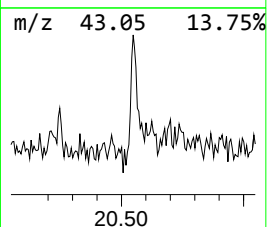
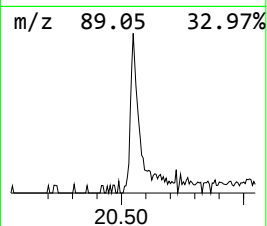
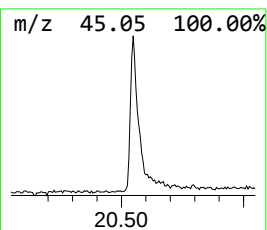
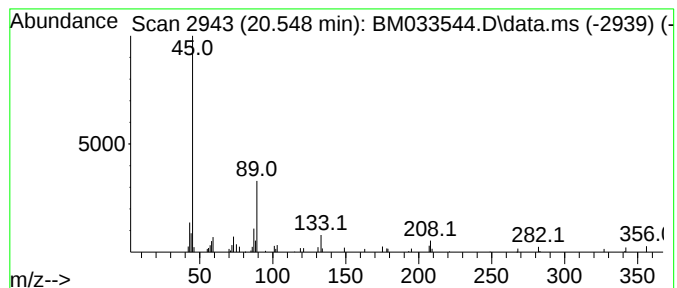
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Peak Number 5 Hexaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.548	3.57 ng	60726	Chrysene-d12	21.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	87
2			Pentaethylene glycol	238	C10H22O6	004792-15-8	80
3			2-[2-[2-[2-[2-(2-Methoxyethox...	340	C15H32O8	004437-01-8	59
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	56
5			1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	56



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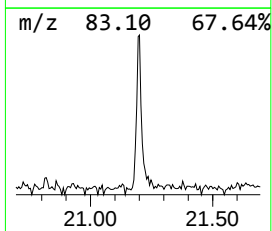
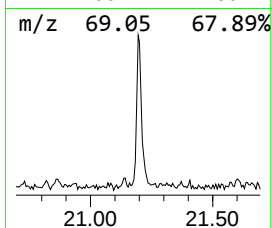
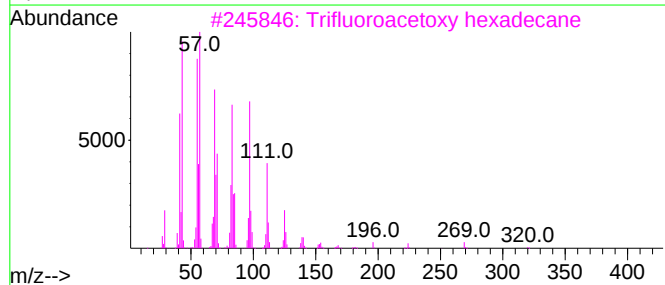
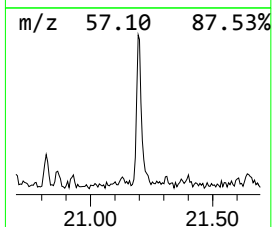
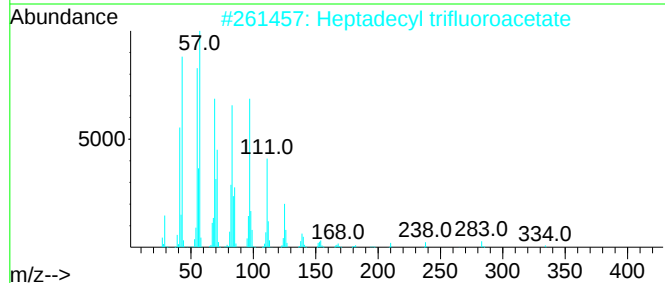
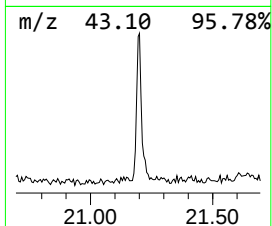
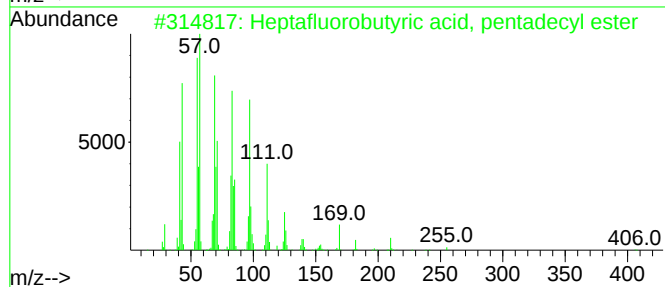
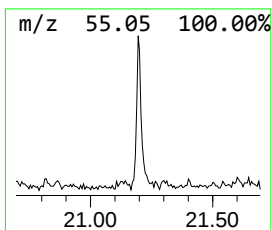
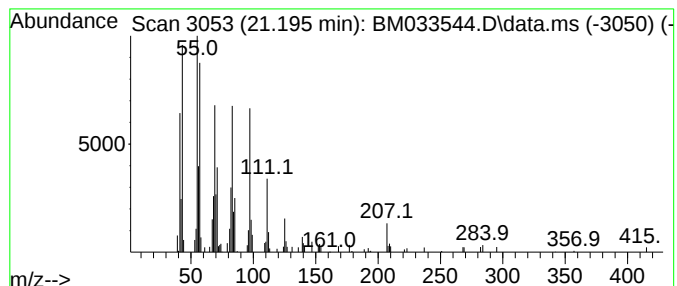
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.195	6.27 ng	106604	Chrysene-d12	21.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033544.D
Acq On : 20 Dec 2021 17:32
Operator : CG/JU
Sample : M5079-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
338

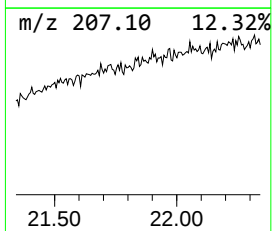
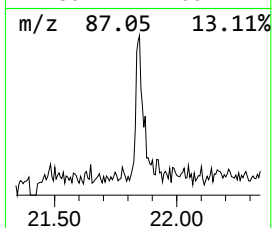
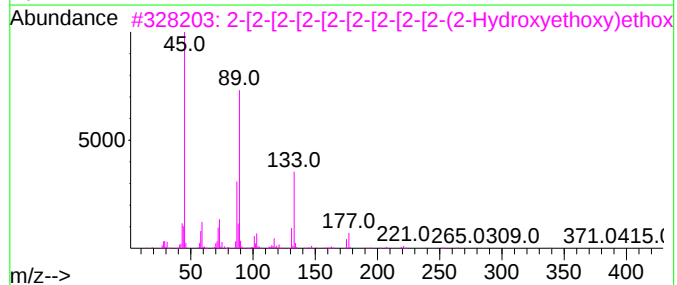
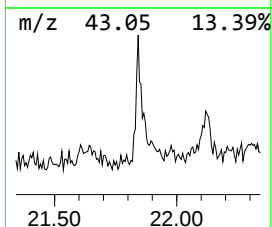
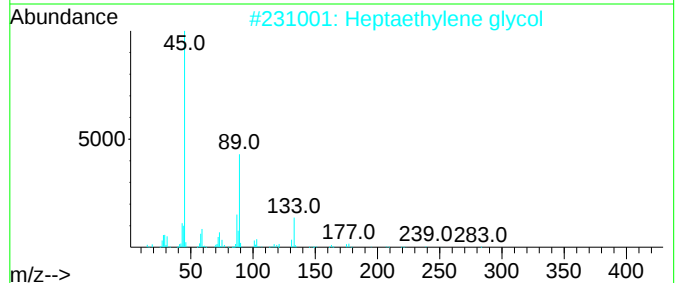
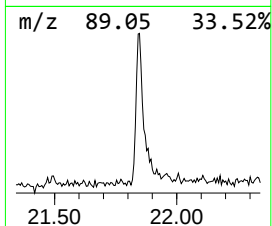
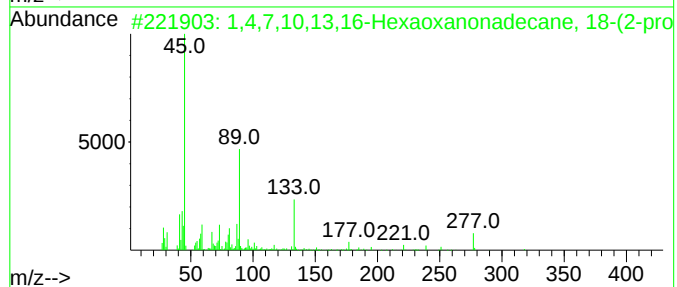
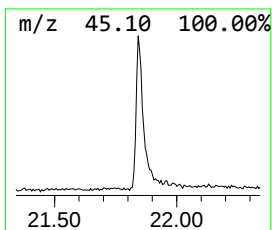
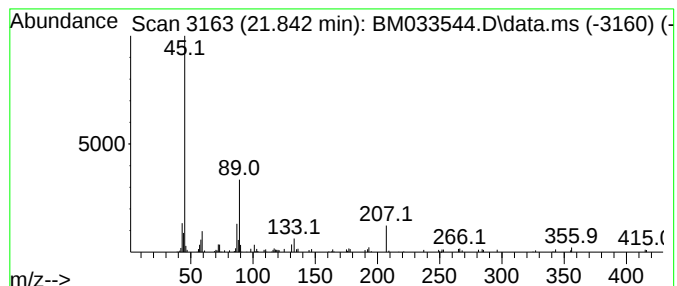
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4,7,10,13,16-Hexaoxonad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.842	4.43 ng	75240	Chrysene-d12	21.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16-Hexaoxonadecane...	318	C16H3006	1000163-64-0	72		
2	Heptaethylene glycol	326	C14H3008	005617-32-3	72		
3	2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42011	005579-66-8	72		
4	Tetraethylene glycol	194	C8H1805	000112-60-7	72		
5	Tetraethyleneglycol monomethylether	208	C9H2005	023783-42-8	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033544.D
Acq On : 20 Dec 2021 17:32
Operator : CG/JU
Sample : M5079-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
338

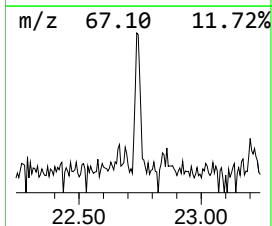
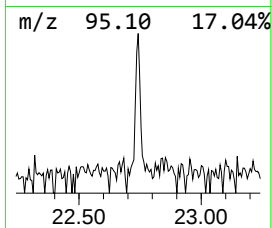
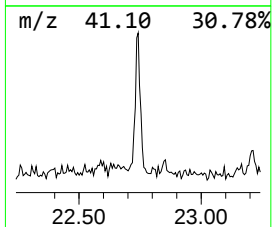
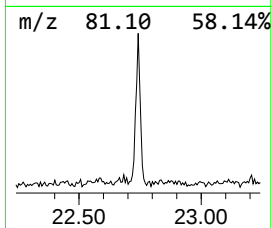
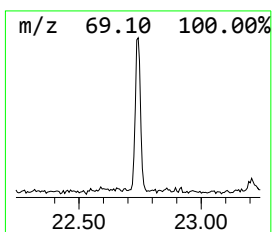
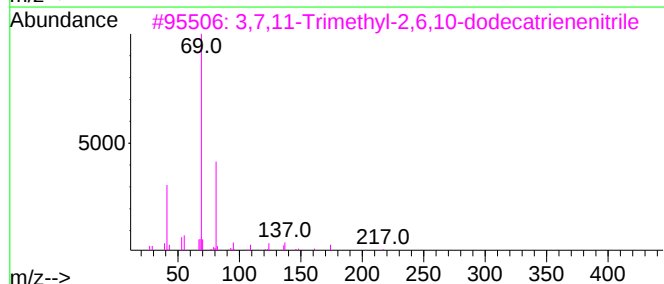
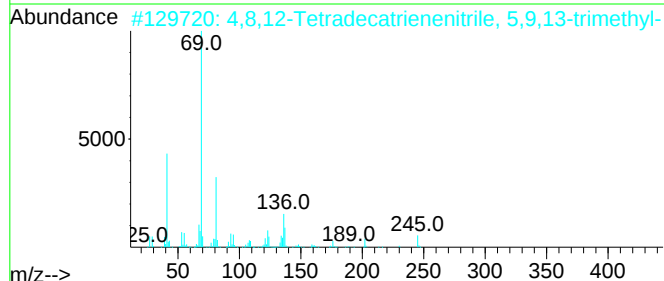
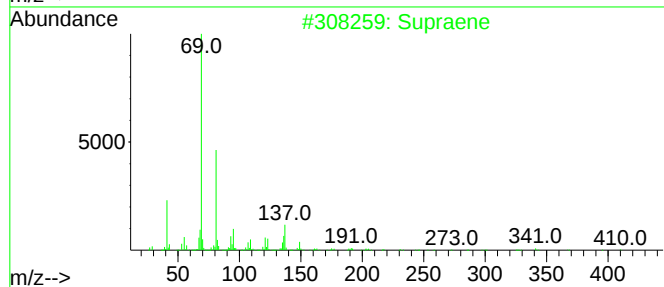
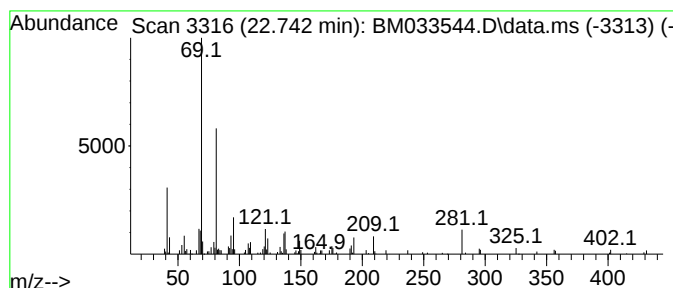
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.742	4.39 ng	70984	Perylene-d12	23.901

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	72
2			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59
3			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	59
5			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033544.D
Acq On : 20 Dec 2021 17:32
Operator : CG/JU
Sample : M5079-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
338

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	3.625	30.3	ng	292786	1	7.919	193378	20.0
2-Pentanone, 4-...	5.025	10.2	ng	98204	1	7.919	193378	20.0
Ethanol, 2-(2-b...	10.525	3.7	ng	46804	2	10.731	250390	20.0
n-Hexadecanoic ...	18.207	3.7	ng	63902	4	17.319	347480	20.0
Hexaethylene gl...	20.548	3.6	ng	60726	5	21.495	339832	20.0
Heptafluorobuty...	21.195	6.3	ng	106604	5	21.495	339832	20.0
1,4,7,10,13,16-...	21.842	4.4	ng	75240	5	21.495	339832	20.0
Supraene	22.742	4.4	ng	70984	6	23.901	323447	20.0